Tutorial on Monte Carlo Simulations – Day 4

Now that your program is working and is optimized, you can compute expectation values of physical observables, which can then be compared to the exact solution in the case of the simple harmonic oscillator.

Following the steps in the first lecture (look for "QFT as Statistical Mechanics" in Andreas's slides, e.g. at `http://theory.fnal.gov/people/kronfeld/ICTP-SAIFR/`), we can relate the statistical average of $A(x)$ in the probability distribution $\exp(-S)$ to the expectation value of the operator $\hat{A}(\hat{x})$ in the ground state of the system

$$\langle A(x_i) \rangle \;=\; \frac{1}{Z} \int \mathcal{D}_x \, A(x_i) \, e^{-S(x_i)} \to \langle 0 | \hat{A} | 0 \rangle$$

when the limit of large $T = Na$ is taken.

Do your results for $\langle x \rangle$, $\langle x^2 \rangle$, $\langle S \rangle$ agree with the expected values?

Similarly, the two-point function $C(t) \equiv \langle x_t \, x_0 \rangle$ we computed last time yields an estimate of the energy of the first excited state

$$\langle x_0 \, x_j \rangle \;=\; \sum_{n \neq 0} |\langle 0 | \hat{x} | n \rangle|^2 \left[e^{(E_n - E_0)\, ja} \;+\; e^{(E_n - E_0)\,(T - ja)} \right]$$

Other Problems

The same program may now be used, with little change, to study the anharmonic oscillator!